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Hybrid Lagrangian-Eulerian Model of HydroGeoChemical Transport

Description

LEHGC is a Lagrangian-Eulerian finite-element model of hydrogeochemical transport through saturated/unsaturated media. LEHGC solves a set of two-dimensional, partial differential equations describing transport with a hybrid Lagrangian-Eulerian finite-element method. The Lagrangian approach to solving the advective component of transport involves single-step node tracking and has been found to be superior to the strictly Eulerian finite-element method in advection-dominated problems.

LEHGC solves a system of transport and geochemical equilibrium equations that are separated into two subsystems which are solved in an iterative fashion. The transport equations, initial and boundary conditions, and the geochemical equilibrium equations govern the migration and chemical reactions of multicomponent species in saturated/unsaturated media. The transport equations include terms for advection, dispersion, diffusion, sources/sinks, and mass production/reduction from radioactive decay and chemical reactions. The chemical reactions considered are aqueous complexation, adsorption/desorption, ion exchange, precipitation-dissolution, redox, and acid-base reactions.

The treatment of chemical equilibrium is based on the equilibrium constant approach which produces a set of nonlinear algebraic equations based on the law of mass action and the principle of mass balance. The aqueous and complexed species are subject to hydrologic transport; the adsorbed, ion-exchanged, and precipitated species are not, and their transport equations do not include terms for advection, dispersion and diffusion. The set of nonlinear, algebraic equations that define the geochemical equilibrium reactions is solved with the Newton-Raphson iterative technique. This set of equations is solved independently at each computational node, at every time step. Because the solution time sometimes monopolizes the CPU time, a massively-parallel version of LEHGC was produced.

Although hydrologic transport is addressed, flow equations are not solved by LEHGC. Rather, the velocity and moisture content fields are either specified as constants in the ASCII input file or read from an external binary file. This binary file may be produced by any flow code and may contain a steady-state solution or transient results over any number of time planes. Flow fields for saturated or unsaturated flow in porous or fractured media can be used in LEHGC simulations. The User's Manual for LEHGC1.1 is available from Sandia (SAND95-1121).

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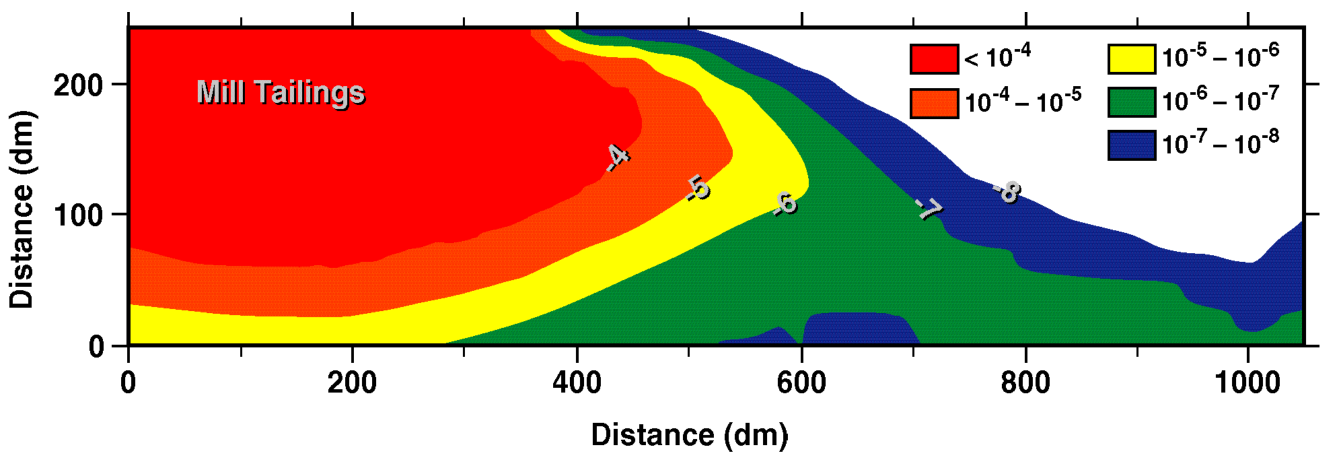
Use of LEHGC in Groundwater Transport/Risk Assessment and Remediation Design

Coupled chemical reaction/transport codes like LEHGC are the only codes that can simulate changes in adsorption and precipitation due to dynamic evolution of the groundwater in response to chemical reactions with the surrounding media. Chemical reactions at the waste source could have profound effects on the transport of toxic metals in the far-field. For example, complex chemical behaviors such as multiple dissolution-precipitation fronts, elevated releases of heavy metals from secondary enrichments, and large variations in K_ds over time could occur. Such phenomena cannot be simulated by available transport or performance assessment codes. LEHGC can be used to enhance our understanding of the fate and transport of mixed and radioactive contaminants in the subsurface and their response when specially formulated chemical additives are introduced. The code can be used to identify inorganic and biogeochemical reactions that sequester or degrade contaminants, understand colloid- or complex-associated contaminants, and quantify the impact of geologic hetergeneity on the effectiveness of various remediation strategies. Using the results of experimental studies of chemical behavior of actinides in groundwater systems and field data from candidate sites, design calculations can be caried out in support of reactive barrier design and evaluation of the efficacy of natural attenuation.



LEHGC was used to simulate uranium transport under changing chemical conditions from a uranium mill tialings pond on the side of a hill. Concentrations of uranium are given in moles/liter.

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